Relativistic Ultrafast Electron Diffraction and Imaging

Tim Noakes
(on behalf of the RUEDI team)

https://ruedi.uk/

Science and Technology Facilities Council
UNIVERSITY OF LIVERPOOL
The Rosalind Franklin Institute
Swansea University Prifysgol Abertawe
UNIVERSITY OF LEEDS

Contents

The RUEDI Project

Lead institute *(University of Liverpool – Prof. Nigel Browning)*
And main partners: *(RFI – Prof. Angus Kirkland)*

UNIVERSITY OF LIVERPOOL

The Rosalind Franklin Institute

UKRI Science and Technology Facilities Council
Daresbury Laboratory

The Materials Innovation Factory

Harwell Campus Hub

Cockcroft Institute

Other science theme leads:

Swansea University Prifysgol Abertawe

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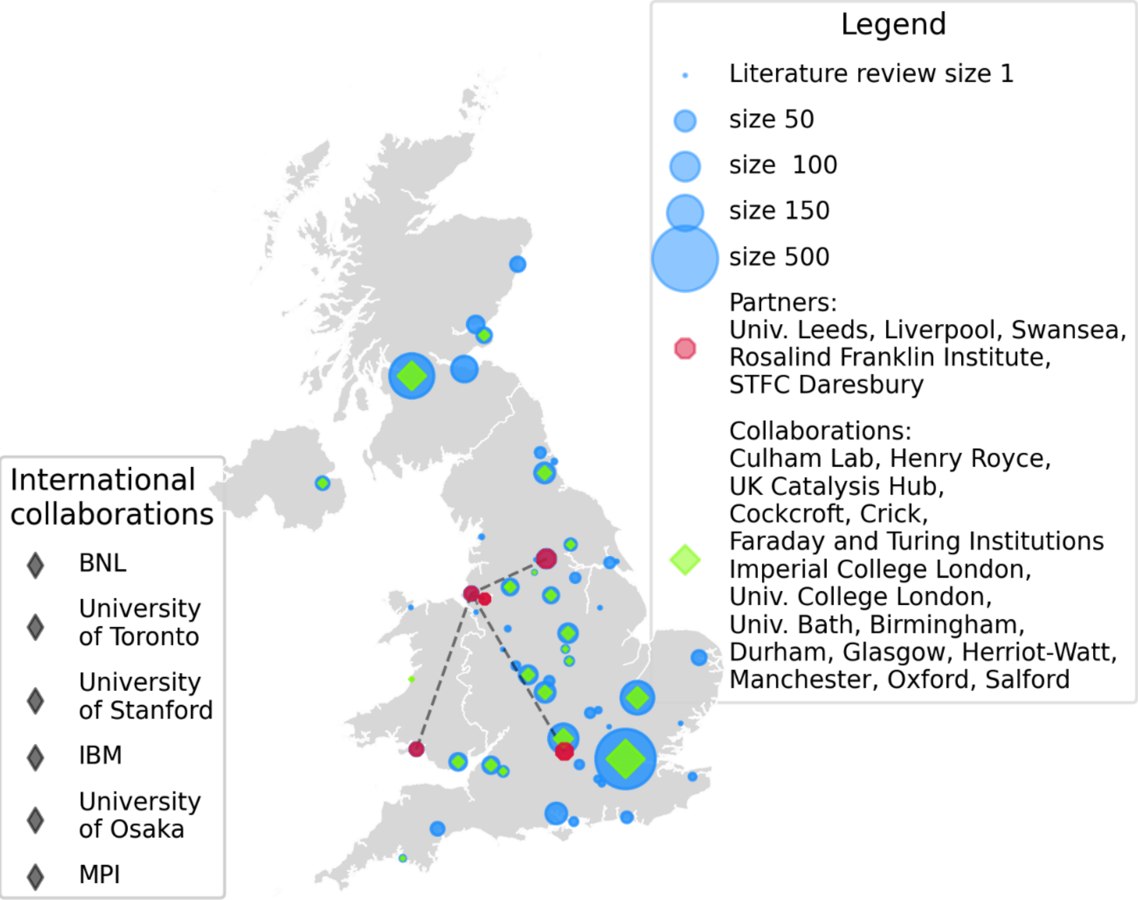
UK Infrastructure Fund:

UKRI UK Research and Innovation

UKRI Engineering and Physical Sciences Research Council

RUEDI collaborations and potential users



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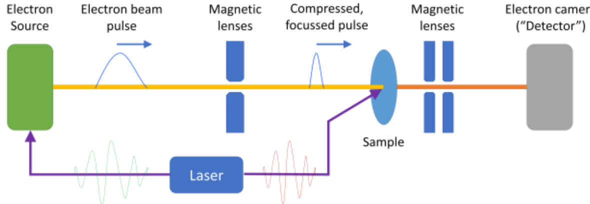
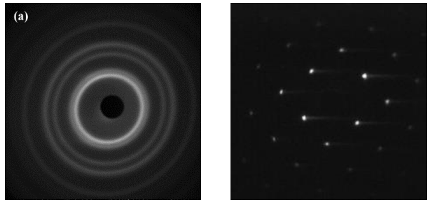
The RUEDI Facility Proposal

- Proposal for a new UK National User Facility
- Relativistic Ultrafast Electron Diffraction & Imaging (RUEDI)



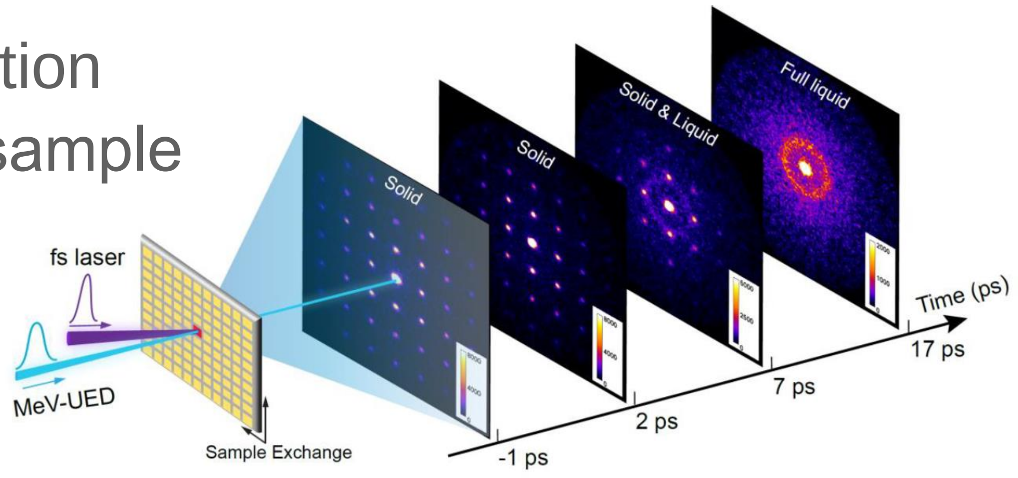
- MeV UED ***and*** UEM
- Time-resolved pump-probe experiments in both real ***and*** reciprocal space
- With a large variety of pumps and sample environments
- To enable a large range of science



- Pumps:
  - Wide variety of laser wavelengths, THz, TW, keV ion source
- Environments:
  - Solid, liquid cells, liquid/gas jets, plasmas, cryogenic (down to mK level)

Pump-probe experiments

- In RUEDI experiments some change is affected by an external stimulus (e.g. laser pump)
- Sample then probed by electron beam
- Variable delay between pump and probe to observe the process in real time
  - Diffraction – provides structural information
  - Imaging – Microscope ‘pictures’ of the sample



“the equivalent of watching a whole game of football rather than just checking the final score”

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Enabling Science

- Town hall meetings held throughout 2022
- Identified experiments, electron parameters, pump sources and sample environments

Mostly Diffraction

- Dynamics of Chemical Change
  - Chemical complexity across scales
  - Hydrogen bonding
  - Pulse radiolysis
  - Heterogenous catalysis

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- Quantum Materials & Processes
  - Ultrafast low-energy optical switching
  - Magnetic textures & skyrmions
  - Topological superconductors
  - Thermoelectric energy harvesting

Swansea University
Prifysgol Abertawe

Mostly Imaging

- Biosciences
  - Photosynthesis & energy transfer
  - Cardiac disease related dynamics
  - Virology & infection
  - Biological self-assembly/toxicity

The Rosalind Franklin Institute

- Materials in Extremes
  - Astrophysics & warm dense matter
  - Advanced manufacturing
  - Nuclear fission/fusion/space
  - Response to shocks

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- Energy Generation, Conversion & Storage
  - Photocatalysis & induced electro-chemistry
  - Defect kinetics in solar cells
  - Ion solvation kinetics in batteries
  - Kinetics of glasses

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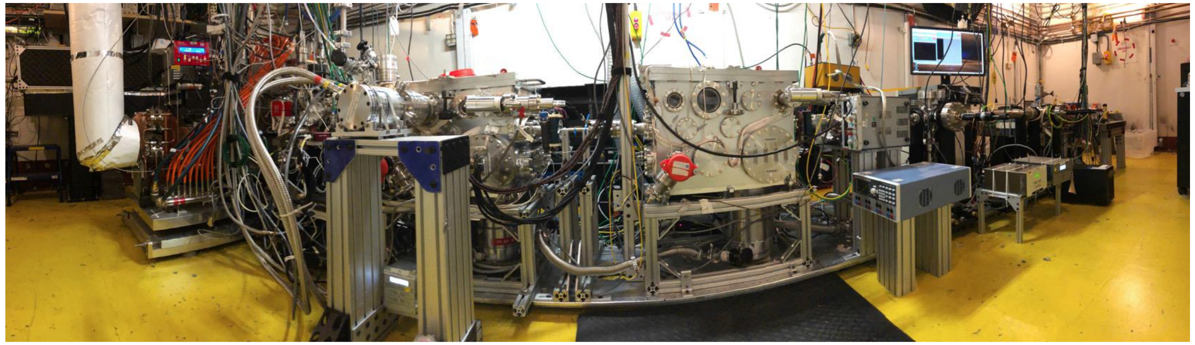
Existing Instruments

- Ultrafast Diffraction
  - Probes structure of materials
  - Based on similar accelerator and laser technology to CLARA and X-FELs
  - Other existing MeV instruments around the world – SLAC/KAERI(Korea)/DESY/Shanghai etc



SLAC MeV UED facility

- Imaging/Microscopy
  - Directly view materials nm-scale
  - Commercial systems at keV level
  - Static (DC) MeV machines – only a few, decades old
  - Higher energy means thicker, more realistic samples
    - Eg/ live cells in liquid instead of frozen
    - Solid-liquid interface in batteries
  - No other MeV time-resolved machine worldwide

Osaka 3 MeV TEM

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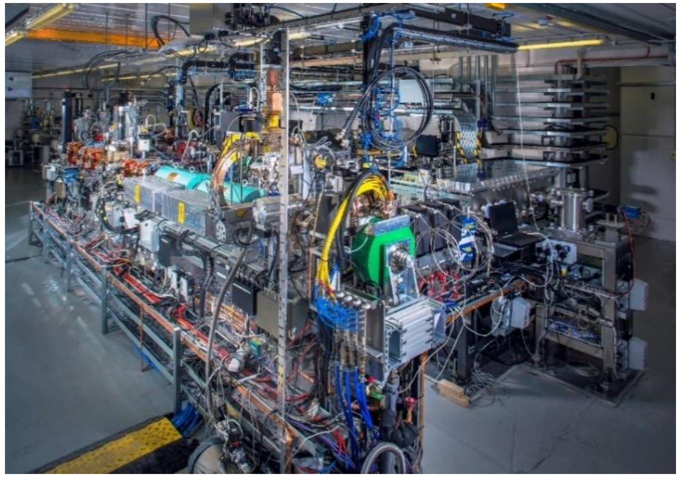
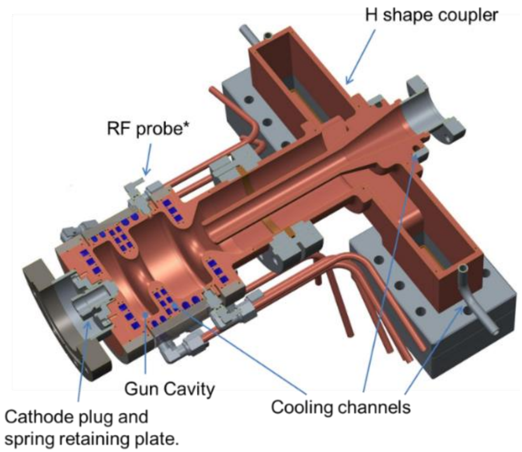
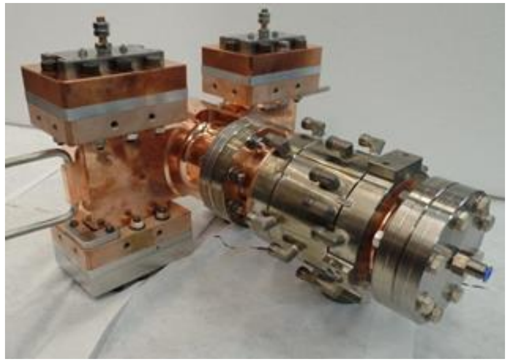
Leveraging ASTeC Experience

Design, build, and operation of particle accelerator facilities

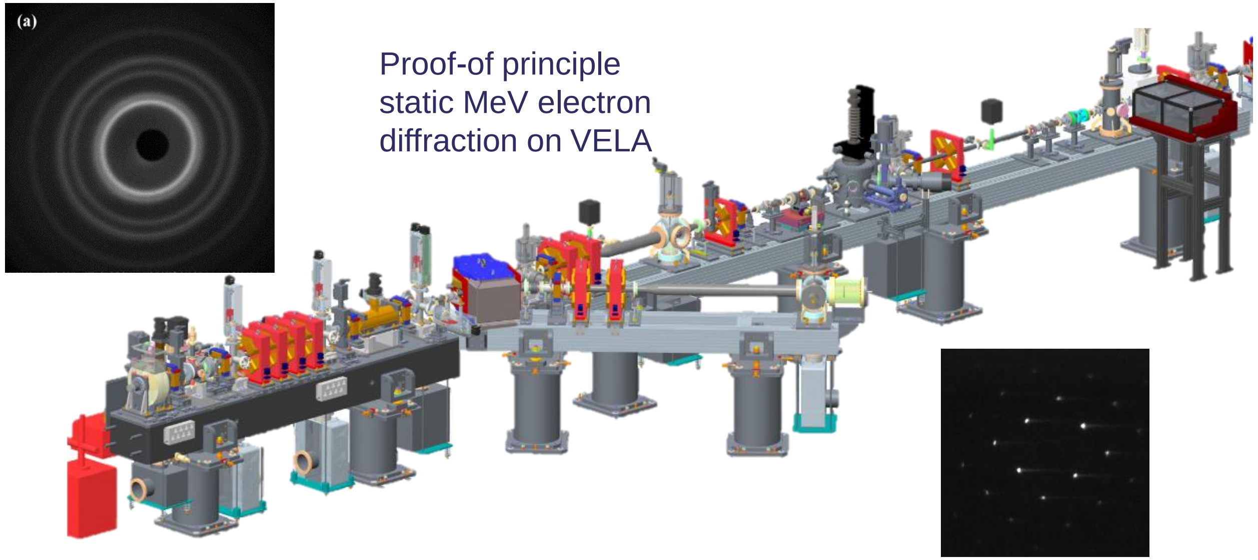


Femtosecond photoinjector development





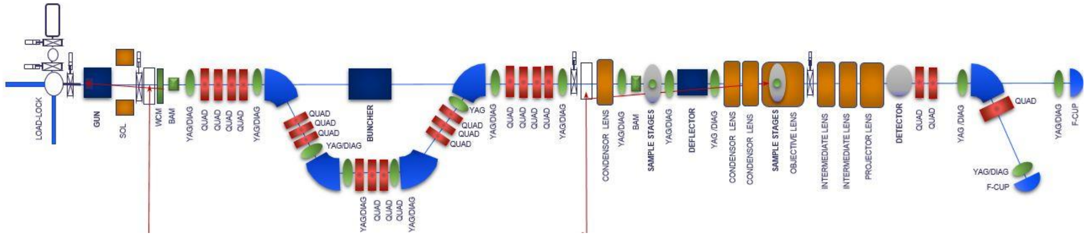
MeV UED Experience



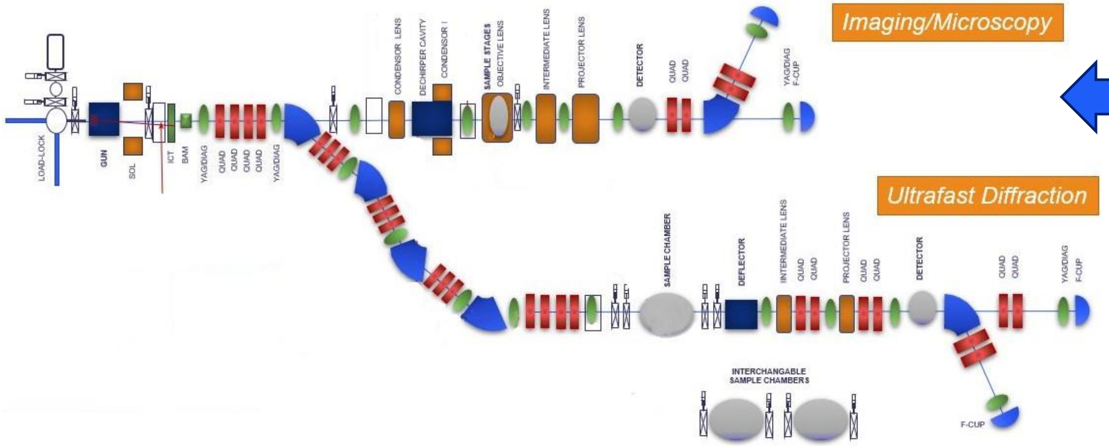
Proof-of principle static MeV electron diffraction on VELA

Instrument Design - Evolution

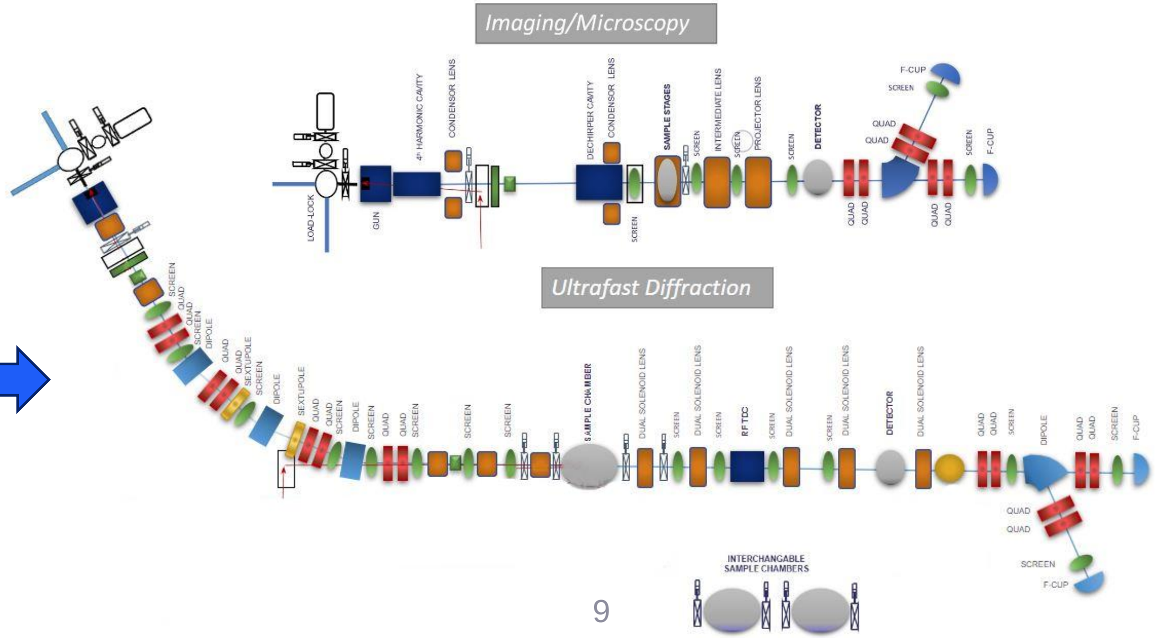
- Initial concept – single beamline for both imaging and diffraction



- Need for different sample stages and environments as well as different beam parameters – one and a half beamline design



- Remove constraints of one beamline on the other to improve performance – current two beam line design

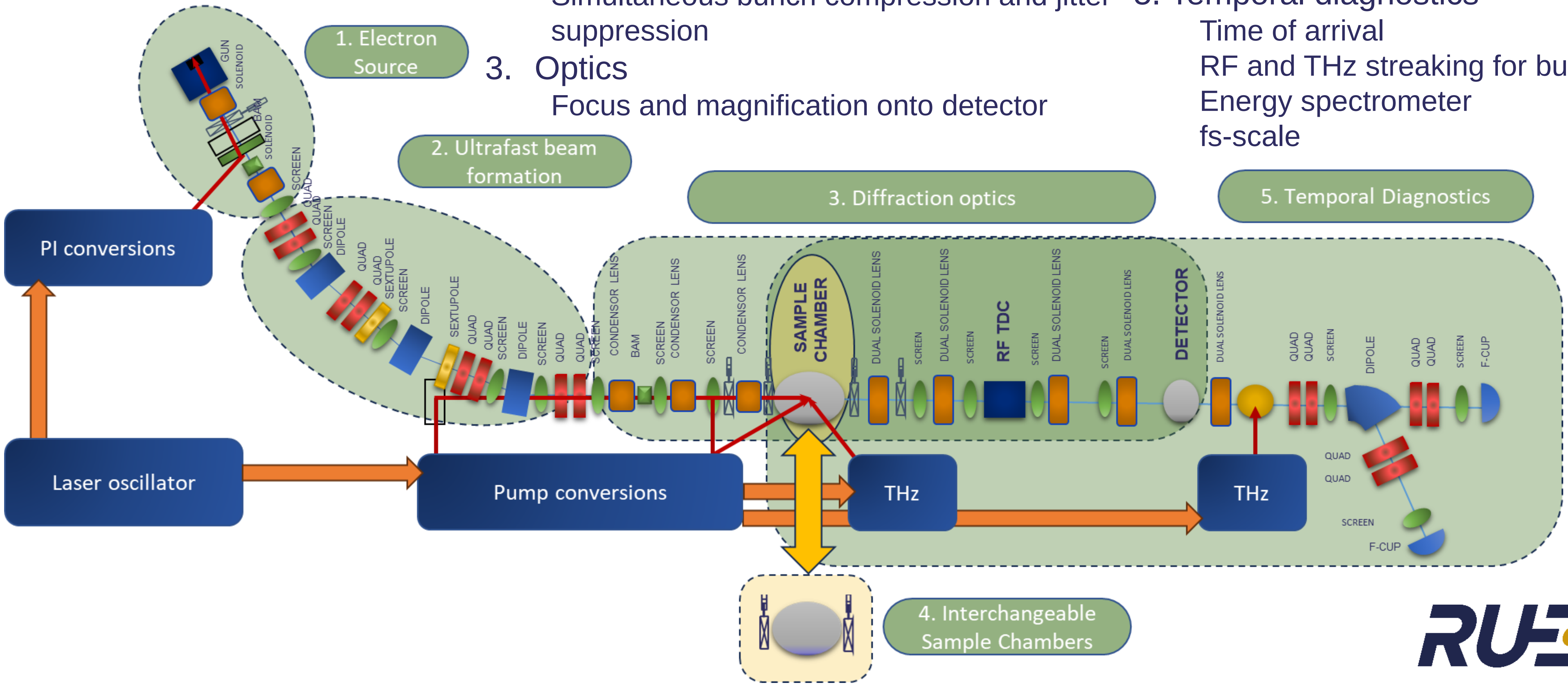


- Laser and RF infrastructure still shared!

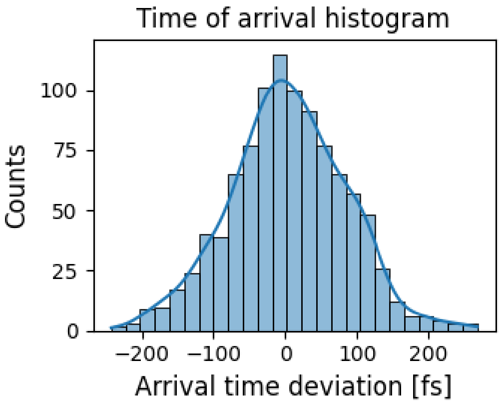
Ultrafast Diffraction Line

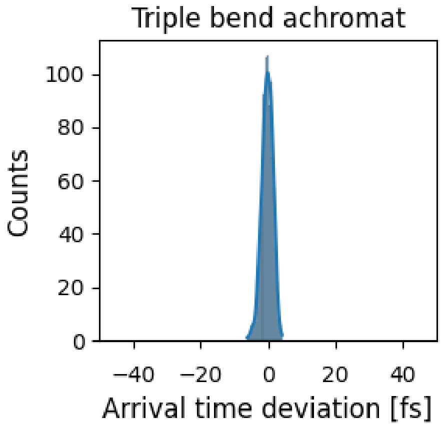
1. S-band RF gun
   Creates high brightness, short pulse beams
2. Magnetic arc
   Simultaneous bunch compression and jitter suppression
3. Optics
   Focus and magnification onto detector

4. Chambers
   Solid, liquid and gas samples
   mK low temperature chamber
5. Temporal diagnostics
   Time of arrival
   RF and THz streaking for bunch length
   Energy spectrometer
   fs-scale

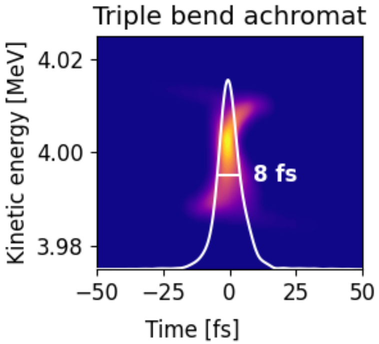


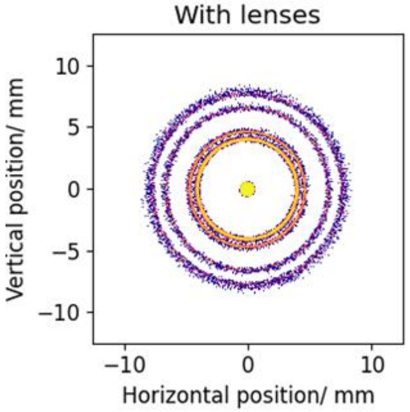
Diffraction Line

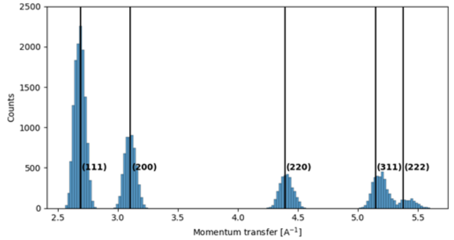


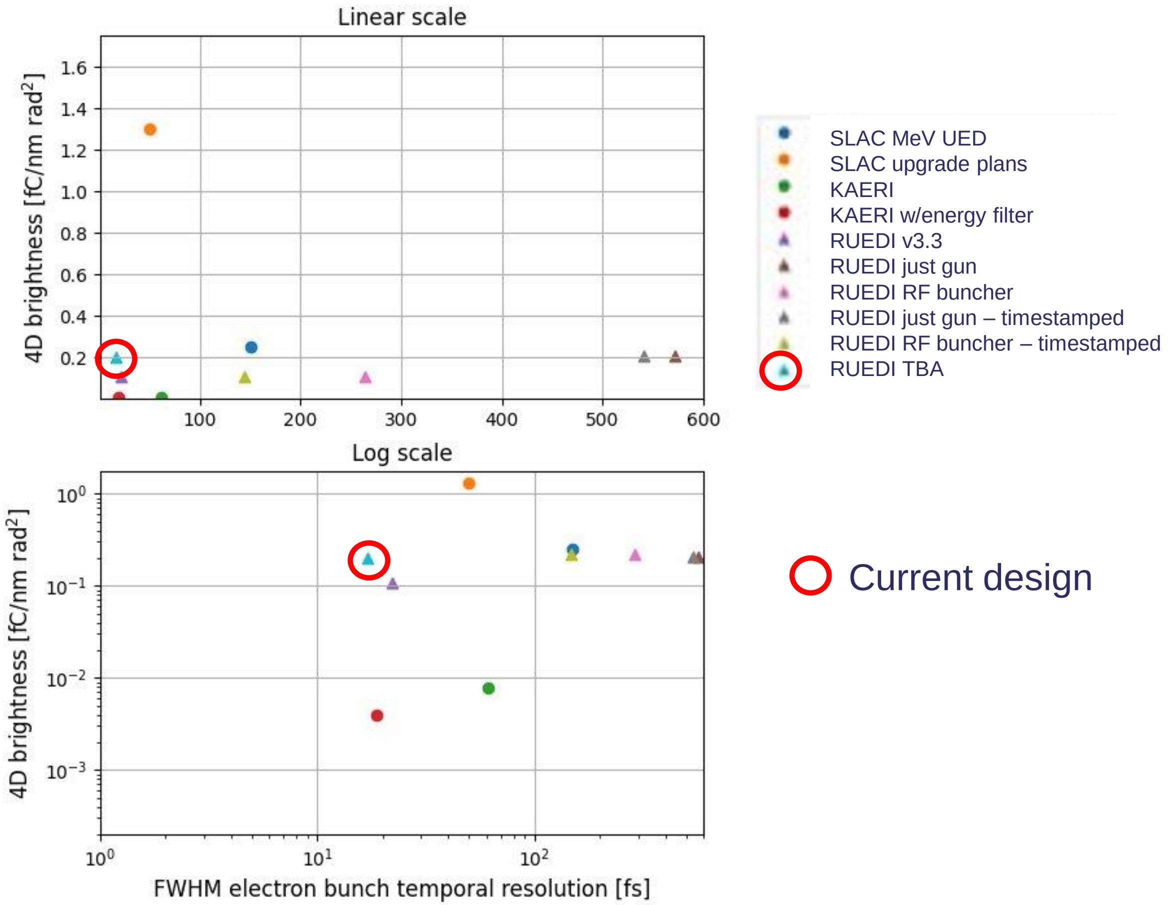


Jitter suppression
(note different scales!)









- Current design suggests
  - 8 fs FWHM timing resolution
  - Excellent transverse resolution for diffraction pattern (related to 4D brightness)
- World-leading performance!

For more information on diffraction line see Ben Hounsell's talk!

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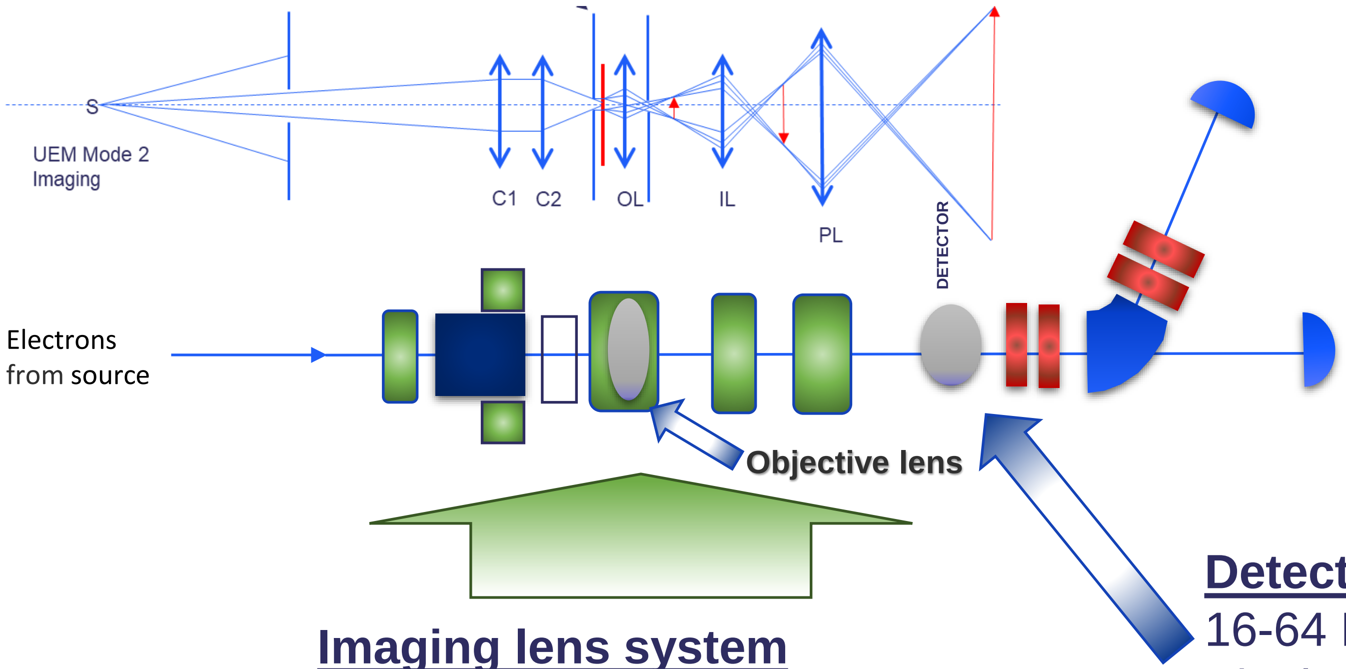
Imaging Beamline



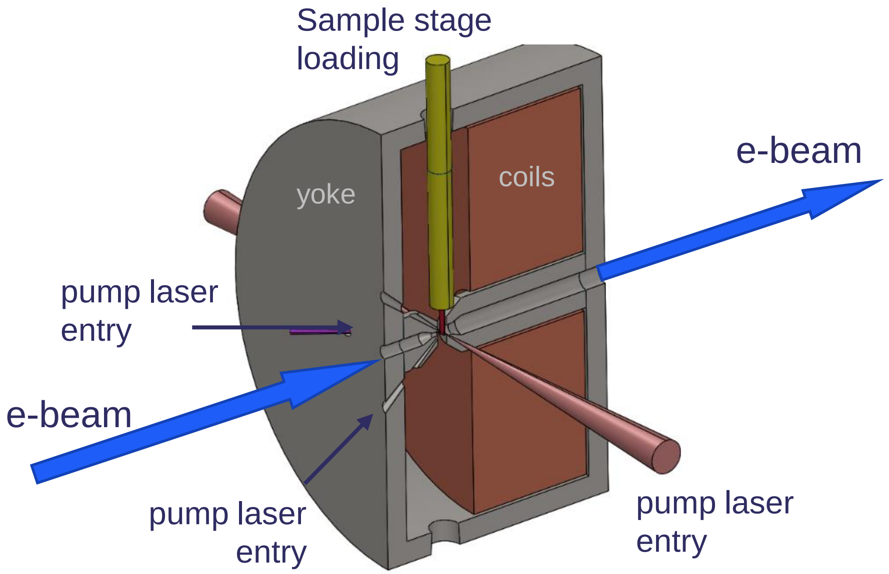
Imaging lens system
Series of magnetic lenses
Aiming for **~9000x** magnification

Detector
16-64 MP
Single electron sensitive

- Energy limited by objective lens to ~ 2 MeV
  - Aberrations from quadrupole options too high (limits lateral resolution)
- Need large number of electrons (10^8 for single-shot images, less with compressive sensing?)
  - (compared to 10^6 for diffraction)

Objective lens

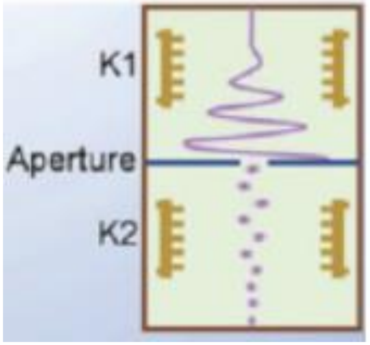
The ***key*** to the whole system



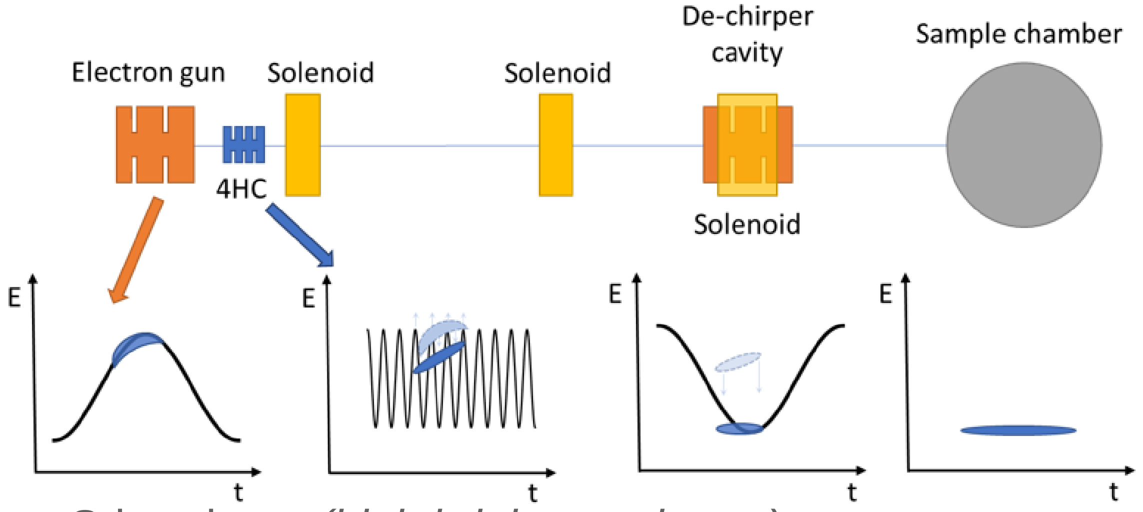
- Samples inserted into middle
- Multiple pump laser entry ports
- Compatible with commercial TEM sample stages (enabling experiments in solid, liquid, cryogenic, heating etc)

Imaging Line – 2 options

- Pulse length determines temporal resolution
- ΔE/E (and lens aberrations) limit imaging resolution
- DC source + fast RF chopper:
  - ΔE/E between 3 x 10^{-5} and 1 x 10^{-6}
  - 10 to 200 ps pulses
  - Maximum 10^4 electrons per pulse (enables stroboscopic use)
  - Bunch trains for 'single shot' (10s of μs resolution only)



- 3 RF cavity beam delivery:
  - ΔE/E between 3 x 10^{-4} and 3 x 10^{-5}
  - Bunch lengths between 0.5 and 12 ps
  - 10^6 to 10^7 electrons per pulse (single-shot may be possible)



- S-band gun *(high brightness beam)*
- 4HC *(lossless monochromation)*
- S-band DCP *(decelerate/dechirp)*

For more information on imaging line see Alex Bainbridge's poster!

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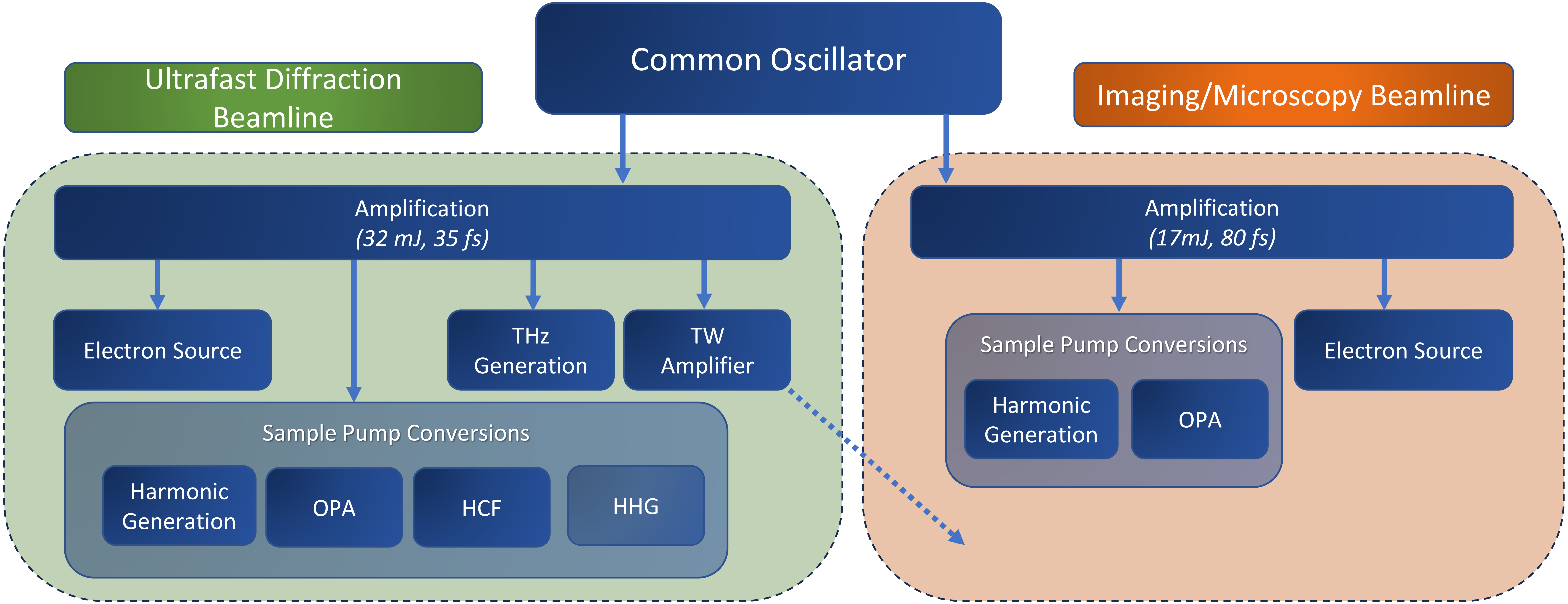
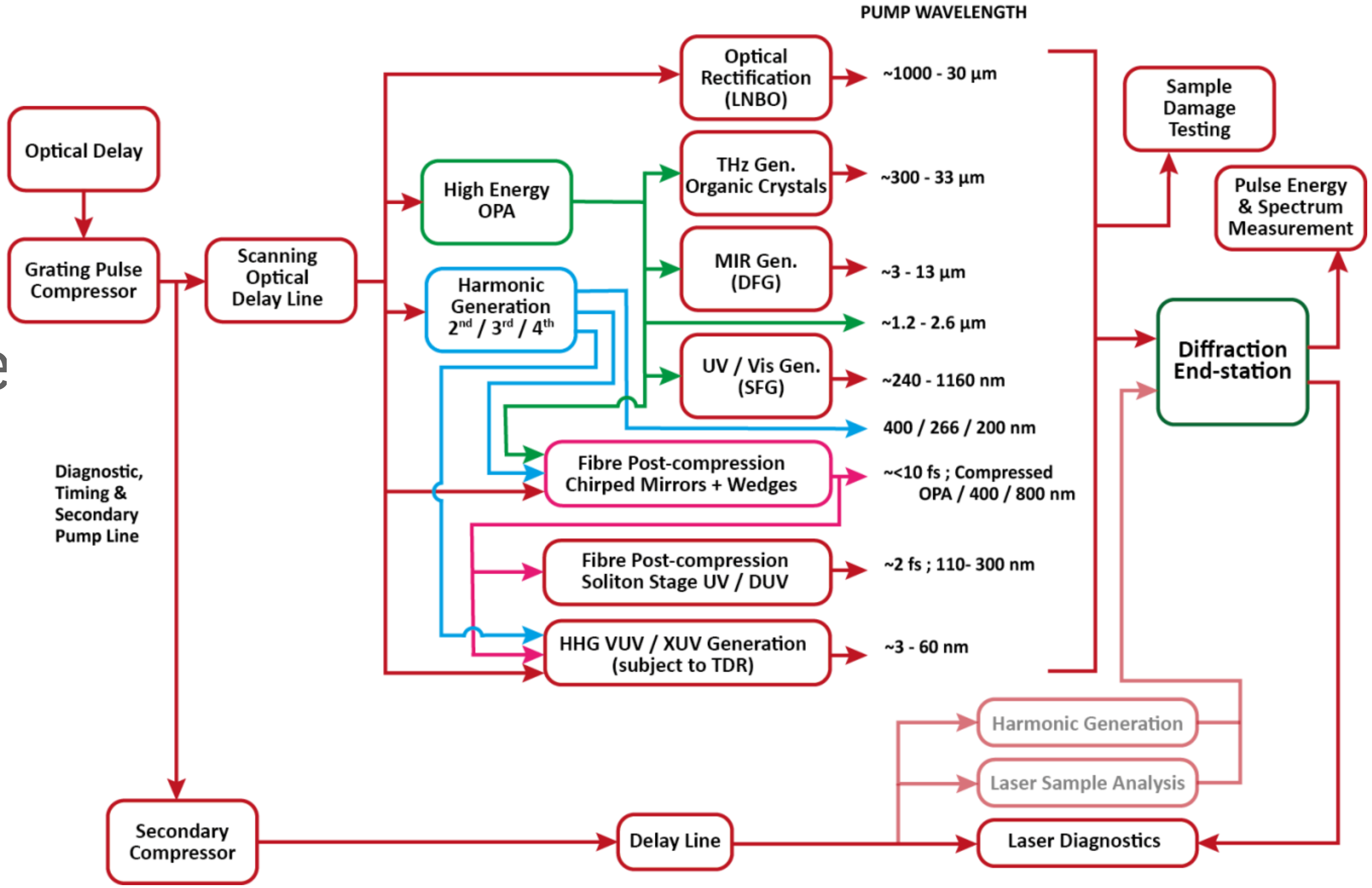
Laser Systems

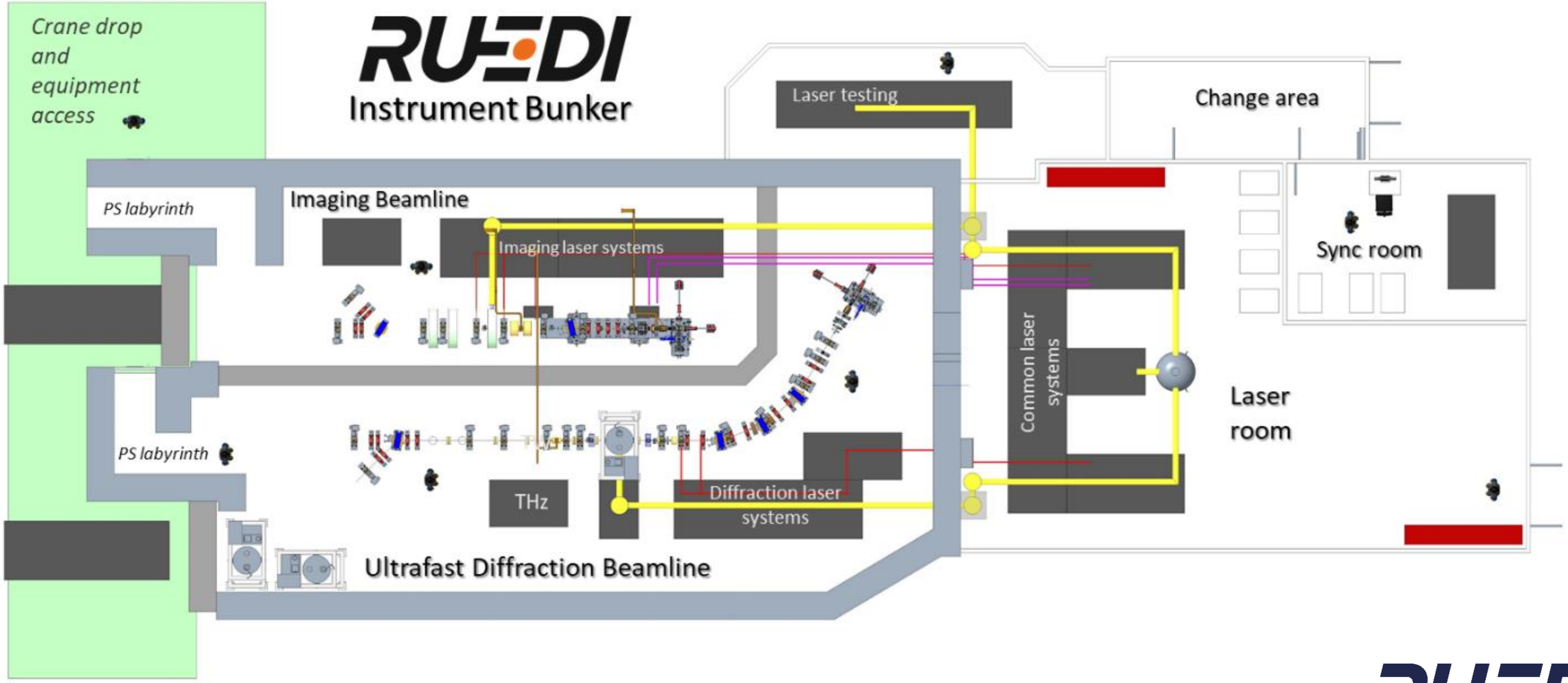


Laser systems

- Proposed experiments demand a wide range of pump lasers
- Both wavelength and pulse length variation required
- Significantly broaden the range of science that can be achieved
  - contribute to the unique capabilities of the instrument/s

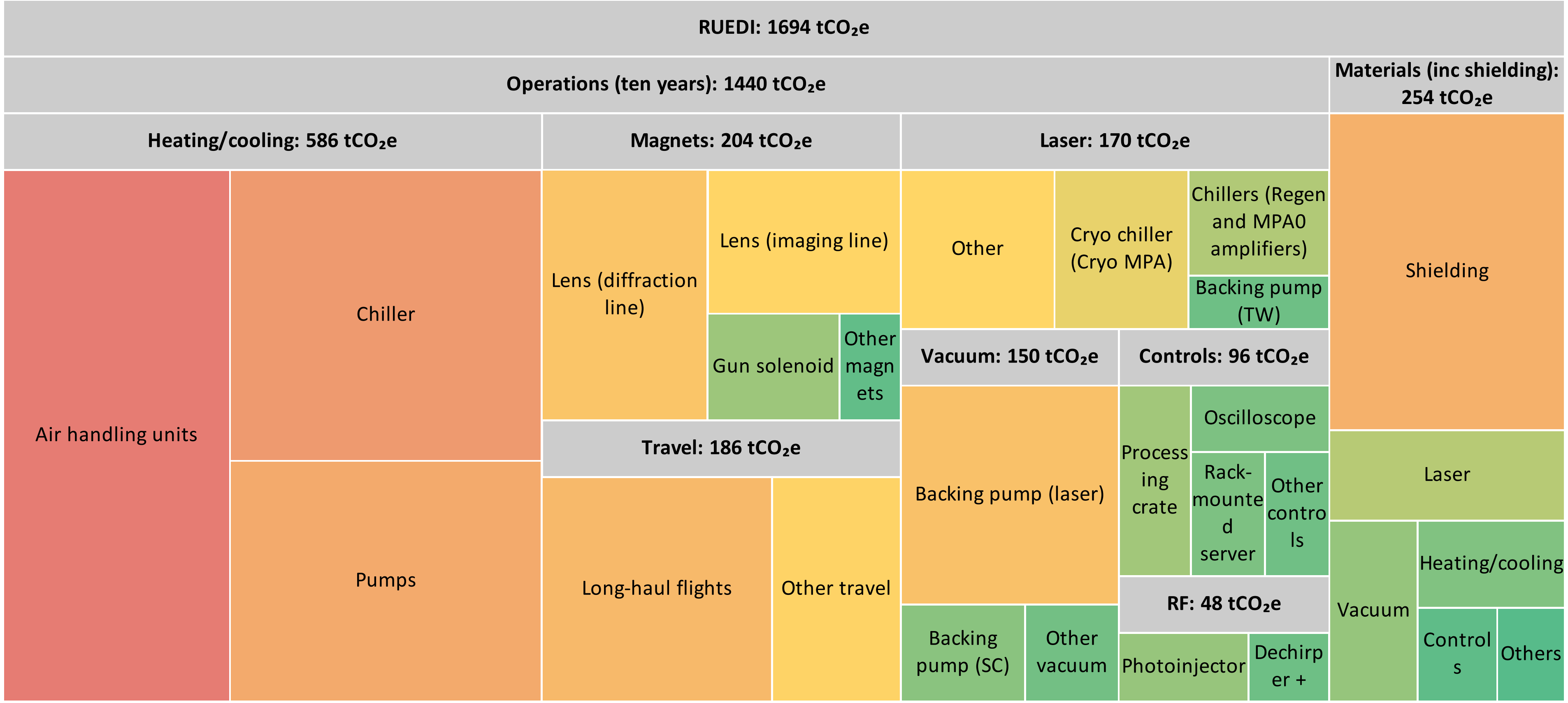


Proposed Layout



Environmental Sustainability

- RUEDI will be the first accelerator designed by ASTeC to fully take sustainability into account



- More in Ben Shepherd's talk later today!

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Digital + Data

- Digital Twin
  - Building on CLARA virtual machine
  - Simulate full user experiments
- AI/Machine Learning integral part of microscope/imaging
  - Reduces number of electrons needed to create single-shot imaging
  - Compressive sensing/inpainting/dictionary learning
- Data challenges
  - 1 kHz rep rate!
  - 16-64 MP detector

Binary readout:

- Unbinned @ 1000 fps = 16.8 Gbps
- Binned @ 1000 fps = 4.2 Gbps

Analog (12-bit) readout:

- Unbinned @ 1000 fps = 201.3 Gbps
- Binned @ 1000 fps = 50.4 Gbps

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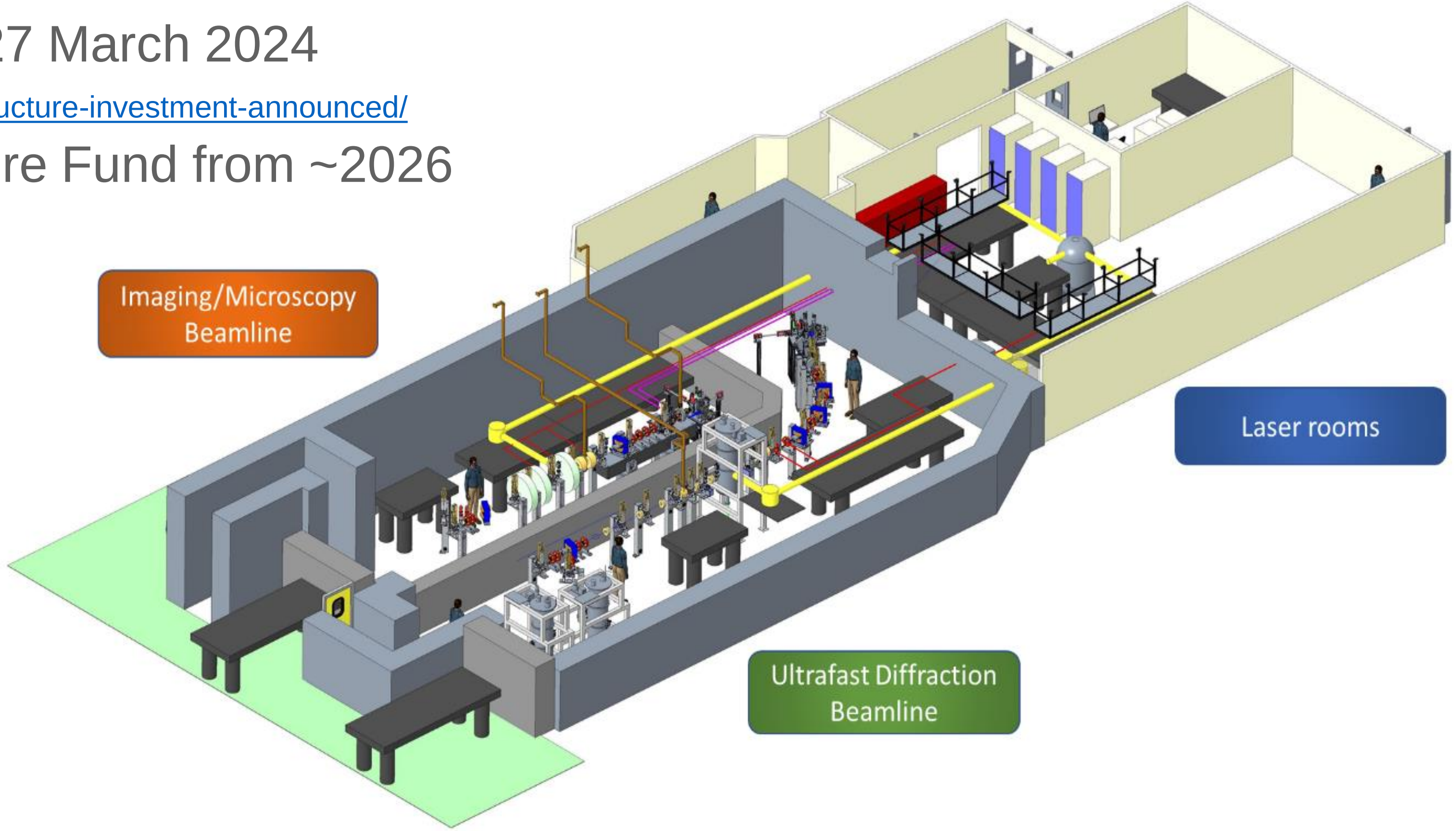
Project status

- Technical design report completed at end of March 2024
- Full project approval announced on 27 March 2024

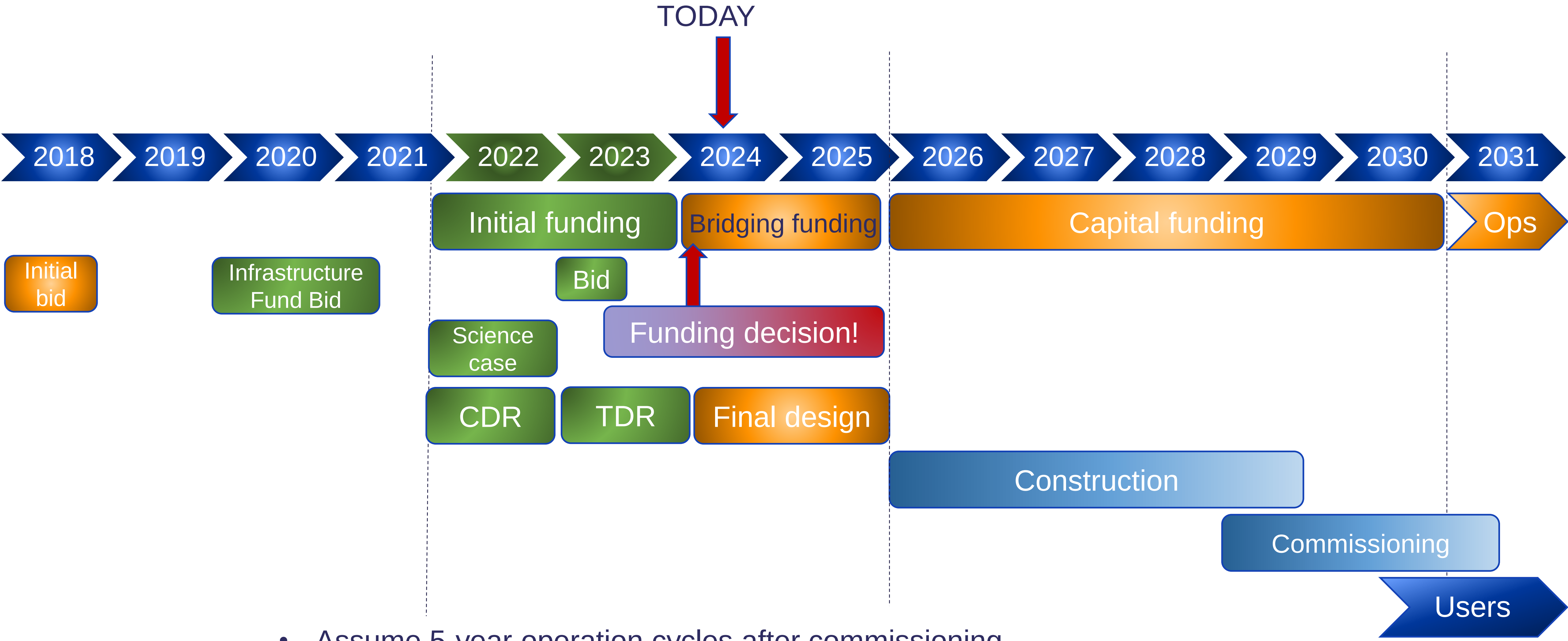
https://www.ukri.org/news/major-research-and-innovation-infrastructure-investment-announced/

- £124.4 million from UKRI Infrastructure Fund from ~2026
  - Subject to full business case approval



- To be sited at Daresbury Laboratory in the Electron Hall, next to CLARA

Timeline



- Assume 5-year operation cycles after commissioning
- Capital for upgrades on same timescales
- At least two 5-year cycles guaranteed!

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Summary

- RUEDI project has received full project approval (£124 M from UKRI Infrastructure Fund)
- Design work is underway
  - Diffraction line will have excellent 4D brightness (diffraction pattern resolution) and world-leading temporal resolution
  - Imaging line still requires more work to deliver single-shot imaging with sub-nm imaging resolution (design choices to be made)
  - Large suite of laser pump sources planned to facilitate diverse science case
  - Environmental sustainability will be key factor in design choices made
- Construction due to commence in 2026, commissioning from 2028 and full user programme from 2030
- For further information
  - Ben Shepherd's talk on sustainability
  - Ben Hounsell's talk on diffraction line
  - Alex Bainbridge's poster on imaging line
  - Suzanna Percival's poster on the diffraction beamline electron source

Acknowledgements

- Thanks to the TDR team!

RELATIVISTIC ULTRAFAST ELECTRON DIFFRACTION & IMAGING (RUEDI) NATIONAL FACILITY

TECHNICAL DESIGN REPORT

VERSION 1.1 [02/04/2024]

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